Refereed Proceedings

The 12th International Conference on Fluidization - New Horizons in Fluidization Engineering

Engineering Conferences International *Year* 2007

Towards Filtered Gas-Solid Flow Models

Juray De Wilde
Université Catholique de Louvain, Belgium,
dewilde@imap.ucl.ac.be

TOWARDS FILTERED GAS-SOLID FLOW MODELS

Juray De Wilde
Materials and Process Engineering Department (IMAP),
Université catholique de Louvain,
Réaumur, Place Sainte Barbe 2, B-1348 Louvain-la-Neuve, Belgium,
T: +32 10 47 8193; F: +32 10 47 4028; E: dewilde@imap.ucl.ac.be

ABSTRACT

To account for meso-scale phenomena in coarse grid simulations, correlation terms appearing in the filtered gas-solid flow equations have to be modeled. Filtered models for the gas-solid momentum transfer are focused on and possible approaches are derived and evaluated. The evaluation supports the combination of an apparent distribution of the filtered gas phase pressure gradient over the phases and an apparent drag force to describe filtered gas-solid momentum transfer. As the filter frequency decreases, the contribution of the apparent distribution of the filtered gas phase pressure gradient over the phases to the filtered description of gas-solid momentum transfer gradually grows in importance up to a mass fraction based distribution, whereas the contribution of the apparent drag gradually vanishes, the mesoscopic description of gas-solid momentum transfer gradually being replaced by a more macroscopic description.

INTRODUCTION

Real fluidized beds contain structures of different length and time scales or different spatial and temporal frequencies ω. The smallest structures that can be calculated using a continuum approach are meso-scale structures, like clusters [1]. Due to the finite spatial and temporal grid dimensions used for solving the continuum gas-solid flow models, a filter frequency ω_f is introduced. The unresolved sub-grid-scale phenomena may affect the lower frequency behaviour explicitly calculated and should, therefore, be accounted for by using so-called filtered models and including sub-grid models [1,2]. The development of sub-grid models is particularly important and complex for gas-solid flows by the intrinsic lack of scale separation in such flows [1,3]. One crucial effect of meso-scale structuring is in the way gas and solids transfer momentum [4]. Therefore, the description of momentum transfer in filtered gas-solid flow models is focused on.

NON-FILTERED MODEL

The Eulerian-Eulerian approach is taken [1,2,5,6]. Expressions for the solid phase physico-chemical properties can be derived from the kinetic theory of granular flow (KTGF) [7]. The transport and constitutive equations used in the present work are discussed in Agrawal et al. [1]. Gas-solid momentum transfer is usually modeled using a drag force term [1,5]. A second contribution to the gas-solid momentum transfer is the distribution over the phases of the gas phase stresses, i.e. the gas phase pressure gradient and/or the gas phase shear stress, according to their volume fraction.

FILTERED MODEL

When performing coarse grid calculations, the gas-solid flow model equations have to be filtered on a scale, i.e. with a filter frequency ω_f, typical for the computational grid that is used. Following Zhang and VanderHeyden [2], Reynolds-averaging is applied to the solids volume fraction and the gas phase pressure, whereas Favre-averaging based on the volume fraction of the phases is applied to the other variables (e.g. $\langle \bar{v} \rangle = \langle \phi \bar{v} \rangle / \langle \phi \rangle$). The filtered model is shown in Table 1.

Filtered mass conservation solid phase:

$$\frac{\partial}{\partial t}\left(\langle\phi\rangle\rho_s\right)+\frac{\partial}{\partial \bar{r}}\cdot\left(\langle\phi\rangle\rho_s\langle\bar{v}\rangle\right)=0 \tag{1}$$

Filtered mass conservation gas phase:

$$\frac{\partial}{\partial t}\left(\langle 1-\phi\rangle\langle\rho_g\rangle\right)+\frac{\partial}{\partial \bar{r}}\cdot\left(\langle 1-\phi\rangle\langle\rho_g\rangle\langle\bar{u}\rangle\right)=0 \tag{2}$$

Filtered momentum conservation solid phase:

$$\frac{\partial}{\partial t}\left(\langle\phi\rangle\rho_s\langle\bar{v}\rangle\right)+\frac{\partial}{\partial \bar{r}}\cdot\left(\langle\phi\rangle\rho_s\langle\bar{v}\rangle\langle\bar{v}\rangle\right)=-\frac{\partial}{\partial \bar{r}}\langle P_s\rangle-\frac{\partial}{\partial \bar{r}}\cdot\left(\langle\phi\rangle\langle\bar{\bar{\tau}}_s\rangle\right)+\langle\phi\rangle\rho_s\bar{g}-\left\langle\phi\frac{\partial P}{\partial \bar{r}}\right\rangle+\left\langle\beta\left(\bar{u}-\bar{v}\right)\right\rangle \tag{3}$$

Filtered momentum conservation gas phase:

$$\frac{\partial}{\partial t}\left(\langle 1-\phi\rangle\langle\rho_g\rangle\langle\bar{u}\rangle\right)+\frac{\partial}{\partial \bar{r}}\cdot\left(\langle 1-\phi\rangle\langle\rho_g\rangle\langle\bar{u}\rangle\langle\bar{u}\rangle\right)=-\frac{\partial\langle P\rangle}{\partial \bar{r}}-\frac{\partial}{\partial \bar{r}}\cdot\langle\bar{\bar{\tau}}_g\rangle+\langle 1-\phi\rangle\langle\rho_g\rangle\bar{g}+\left\langle\phi\frac{\partial P}{\partial \bar{r}}\right\rangle-\left\langle\beta\left(\bar{u}-\bar{v}\right)\right\rangle \tag{4}$$

Table 1. Filtered conservation equations.

By using Favre-averaging, no correlations appear in the mass conservation equations. This is not the case in the momentum equations. Currently, no reliable closure models are available for the convection related correlations. These terms are, however, of minor importance for the present work. Commonly, they are incorporated in the viscous shear terms. In what follows, the closure models for the filtered gas-solid momentum transfer terms are focused on, the last two terms on the right hand side of Eqs. (3) and (4). Recent studies [1,2] on the filtered drag have shown a significant reduction of the drag coefficient by the presence of solid phase meso-scale structures (clusters). To account for the latter in coarse mesh simulations in which the solid phase meso-scale structures are filtered out, a filtered or effective drag coefficient β_e has been introduced to close the filtered or effective drag force [8,9,10]:

$$\left\langle\beta\left(\bar{u}-\bar{v}\right)\right\rangle=\beta_e\left(\langle\bar{u}\rangle-\langle\bar{v}\rangle\right) \tag{5}$$

The filter frequency ω_f is not explicitly accounted for in the β_e-formulations proposed. Andrews et al. [10] investigated both the time-averaged β_e approach (Eq. (5)) and a stochastic correction. Most formulations predict a reduction of the drag coefficient by a factor 1.5 to 4, depending on the filtered solids volume fraction, in agreement with the reduction calculated from dynamic mesoscale simulations on a periodic 2x8 cm^2 domain [1]. With respect to the latter simulations, it should, however, be remarked that the ratio of the domain size used for averaging or filtering and the mesh size is only 32, i.e. only a limited amount of effects is filtered out. Hence, it is possible that for lower ω_f, e.g. in case of steady-state simulations, as more effects are filtered out, the value of β_e is further reduced. In the present work, the β_e-formulation of Heynderickx et al. [9] and the drag coefficient of Wen and Yu [11] reduced with a constant factor, are used for a qualitative sensitivity analysis of the β_e-approach.

The correlation between the gas phase pressure gradient and the solid volume fraction, $\langle \phi' \partial P'/\partial \bar{r} \rangle$, appears from:

$$\left\langle \phi \frac{\partial P}{\partial \bar{r}} \right\rangle = \langle \phi \rangle \left\langle \frac{\partial P}{\partial \bar{r}} \right\rangle + \left\langle \phi' \frac{\partial P'}{\partial \bar{r}} \right\rangle \tag{6}$$

Zhang and VanderHeyden [2] were the first to study the $\langle \phi' \partial P'/\partial \bar{r} \rangle$ term and found it to be surprisingly important. An apparent added mass closure model is proposed:

$$\left\langle \phi' \frac{\partial P'}{\partial \bar{r}} \right\rangle = C_a \langle \rho_m \rangle \left(\frac{\partial \langle \bar{v} \rangle}{\partial t} + \langle \bar{v} \rangle \cdot \frac{\partial \langle \bar{v} \rangle}{\partial \bar{r}} - \frac{\partial \langle \bar{u} \rangle}{\partial t} - \langle \bar{u} \rangle \cdot \frac{\partial \langle \bar{u} \rangle}{\partial \bar{r}} \right) \tag{7}$$

which scales with the volume fraction based mixture density ρ_m and the apparent added mass coefficient C_a for which a formulation as a function of ω_f is yet to be derived. For what follows, the 1D inviscid form of the filtered momentum equations obtained with an apparent added mass approach is given here:

$$\langle \phi \rangle \rho_s \frac{D\langle v \rangle}{Dt} = -\langle \phi \rangle \nabla \langle P \rangle - C_a \langle \rho_m \rangle \frac{D\langle v \rangle}{Dt} + C_a \langle \rho_m \rangle \frac{D\langle u \rangle}{Dt} + \langle \phi \rangle \rho_s g + \langle \beta(\bar{u} - \bar{v}) \rangle \tag{8}$$

$$(1 - \langle \phi \rangle) \rho_g \frac{D\langle u \rangle}{Dt} = -(1 - \langle \phi \rangle) \nabla \langle P \rangle + C_a \langle \rho_m \rangle \frac{D\langle v \rangle}{Dt} - C_a \langle \rho_m \rangle \frac{D\langle u \rangle}{Dt} + (1 - \langle \phi \rangle) \rho_g g - \langle \beta(\bar{u} - \bar{v}) \rangle \tag{9}$$

Zhang and VanderHeyden [2] and De Wilde [12] found that C_a can be much larger than one, resulting in an apparent added mass that is surprisingly large compared to the well-known added mass which is commonly neglected in gas-solid flow simulations.

Neglecting the drag force in Eqs. (8) and (9), De Wilde [12] showed that the apparent added mass can be reformulated in terms of an apparent distribution of the filtered gas phase pressure gradient over the phases. Furthermore, such an apparent distribution of the filtered gas phase pressure gradient over the phases was shown to appear directly from the correlation between the solid volume fraction and the gas phase pressure gradient $\langle \phi' \partial P'/\partial \bar{r} \rangle$ and to scale according to the mean square of the solid volume fraction fluctuations $\langle \phi' \phi' \rangle$:

$$\left\langle \phi \frac{\partial P}{\partial z} \right\rangle = \left[\langle \phi \rangle + \frac{\langle \phi' \phi' \rangle}{\langle \phi \rangle} \left(\langle m_s \rangle - \frac{\langle \phi \rangle \rho_g}{\langle \rho_m \rangle} \right) \right] \left\langle \frac{\partial P}{\partial z} \right\rangle + \left\langle \phi' \frac{\partial \tilde{P}'}{\partial z} \right\rangle \tag{10}$$

, introducing the Reynolds-averaged solids mass fraction $\langle m_s \rangle$.

Because of the large density difference between the phases, Eq. (10) can be simplified to:

$$\left\langle \phi \frac{\partial P}{\partial z} \right\rangle = \left[\langle \phi \rangle + \frac{\langle \phi' \phi' \rangle}{\langle \phi \rangle} \langle m_s \rangle \right] \left\langle \frac{\partial P}{\partial z} \right\rangle + \left\langle \phi' \frac{\partial \tilde{P}'}{\partial z} \right\rangle \tag{11}$$

An indirect contribution to the apparent distribution of the filtered gas phase pressure gradient over the phases resulting from $\langle \phi' \partial \tilde{P}' / \partial z \rangle$ was shown to be statistically significant, but one order of magnitude less important than the direct contribution.

In the next paragraphs, the two approaches for describing filtered gas-solid momentum transfer, i.e. the effective drag approach and the apparent added mass approach, are evaluated based on a mixture speed of sound test. Furthermore, the apparent added mass is reformulated accounting for the presence of the drag force in Eqs. (8) and (9) to analyse its meaning and effects and to improve insight in the filtered description of gas-solid momentum transfer.

MIXTURE SPEED OF SOUND TEST

Filtered models should allow to calculate the low frequency behavior without explicitly calculating the high frequency behavior. Experimental observations show that gas-solid flows exhibit an interesting behavior with respect to frequency

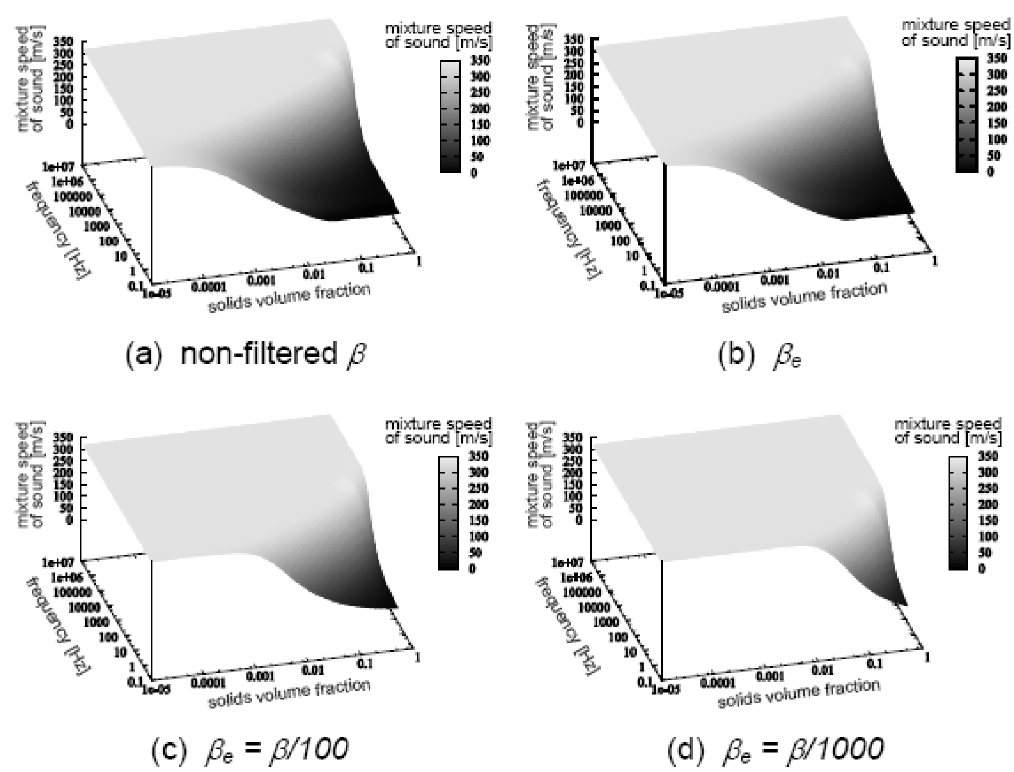

Figure 1. Mixture speed of sound as a function of the wave frequency and the solid volume fraction calculated with the non-filtered and the filtered model (Eqs. (1)-(5)) with: (a) non-filtered β, (b) effective drag coefficient β_e [9], (c) $\beta_e = \beta/100$, (d) $\beta_e = \beta/1000$. Conditions: ρ_s = 2650 kg m^{-3}, ρ_g = 0.934 kg m^{-3}, d_p = 310 µm, $<P>$ = 104800 Pa. (a) → (d): β_e expected to ↓ as coarser grids are used.

dependence. The propagation speed of gas phase pressure waves in gas-solid mixtures, the so-called mixture speed of sound c_m, strongly depends on the solids volume fraction and, more importantly for the present investigation, on the wave frequency [13,14,15].

The complex behavior of c_m is a result of gas-solid momentum transfer. One of the early successes of the non-filtered Eulerian-Eulerian gas-solid flow model was its capability of describing the complex behavior of c_m over the entire solids volume fraction and frequency ranges (Figure 1(a)) [14,15]. Higher frequency pressure waves, typically with a frequency higher than 10^6 Hz, propagate quasi-undisturbed through the gas-solid mixture, i.e. the high frequency mixture speed of sound equals the single gas phase speed of sound c_g. As the frequency decreases, the mixture speed of sound is gradually decreased by the presence of solid particles. At low frequencies, c_m gradually decreases from the single gas phase speed of sound c_g for solid volume fractions lower than 10^{-5} to a minimum mixture speed of sound for solid volume fractions higher than about 0.1.

The gas-solid momentum transfer terms were found to play a crucial role in the calculated c_m-behavior. The frequency dependence of c_m then suggests an interesting test for filtered momentum transfer models. Such models should still be able to describe c_m for frequencies lower than a certain chosen frequency, i.e. the filter frequency ω_f, but not necessarily for frequencies higher than ω_f.

Effective Drag Force Approach

Figure 1 shows a qualitative sensitivity analysis of the mixture speed of sound calculated from the filtered gas-solid flow model (Eqs. (1)-(4)) taking a β_e-approach (Eq. (5)) on the value of β_e. The β_e-approach is seen to affect the mixture speed of sound c_m over the entire frequency range, independent of the value of β_e. In particular, c_m at low frequencies is also altered. Furthermore, as β_e decreases, the high frequency mixture speed of sound behavior is gradually introduced over lower frequencies.

The behavior of the β_e-approach is undesirable for filtered models. If a β_e-approach is taken, another contribution to the filtered description of gas-solid momentum transfer is needed in order to restore the mixture speed of sound behavior at frequencies below a certain chosen frequency, i.e. the filter frequency.

Apparent Added Mass Approach

Figure 2 shows the effect of an apparent added mass approach (Eq. (7)) for $\langle \phi' \nabla P' \rangle$ (Eq. (6)) on the mixture speed of sound behavior calculated from a filtered model. As ω_f decreases and $\langle \phi' \nabla P' \rangle$ grows in importance, C_a is expected to increase. As C_a increases, the mixture speed of sound behavior is progressively affected from the high frequencies on and a filter frequency ω_f can indeed be defined. In fact, the filter frequency mixture speed of sound behavior $c_m(\omega_f)$ is introduced to frequencies ω higher than ω_f. The mixture speed of sound behavior for frequencies ω lower than ω_f is, however, not affected and remains being predicted correctly by the filtered model. As such, the impact of the apparent added mass closure term (Eq. (7)) on the mixture speed of sound behavior calculated from the filtered gas-solid flow model (Eqs. (1)-(4)) is in agreement with the behavior generally expected from filtered models. Figure 2 furthermore teaches that apparent added mass coefficient values

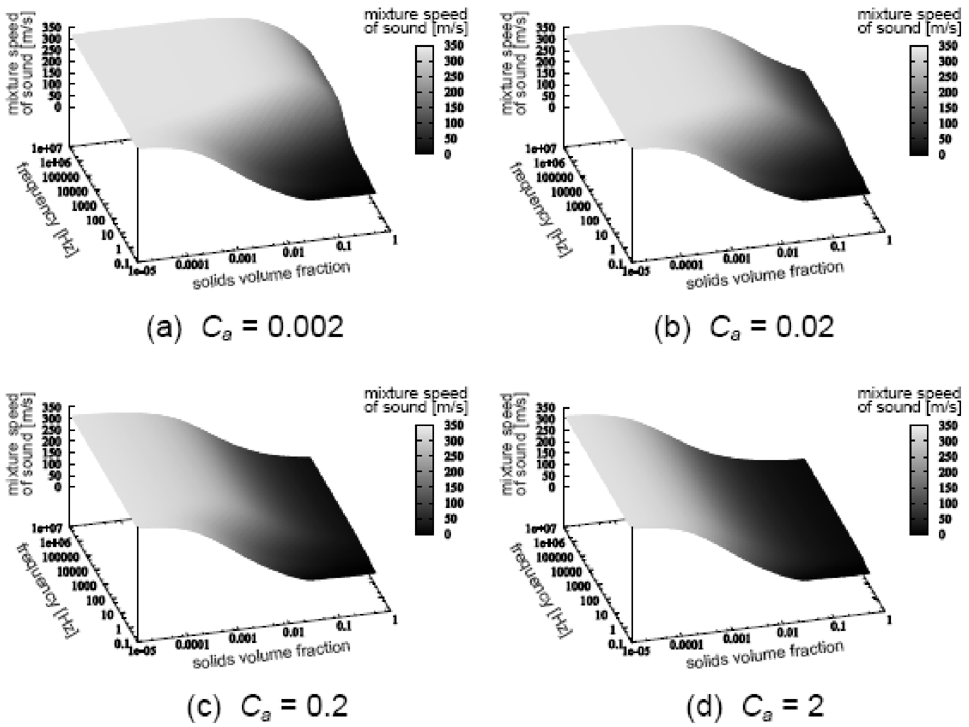

Figure 2. Mixture speed of sound as a function of the wave frequency and the solid volume fraction calculated with the filtered model (Eqs. (1)-(4), (6)-(7)) with an apparent added mass [2,12] with: (a) $C_a = 0.002$, (b) $C_a = 0.02$, (c) $C_a = 0.2$, (d) $C_a = 2$. Conditions: see Figure 1. (a) $\rightarrow$ (d): $C_a \uparrow$ as $\omega_f \downarrow$.

larger than 1, as stated by Zhang and VanderHeyden [2], are indeed possible and allowable for filter frequencies ω_f lower than 10 Hz. Such low ω_f are unlikely to be introduced by spatial filtering, as this would imply mesh dimensions of the order of meters, but are easily introduced by temporal filtering, as for example in steady state simulations.

The effective drag force and the correlation between the gas phase pressure gradient and the solid volume fraction $\langle \phi' \nabla P' \rangle$ (Eqs. (5)-(7)) are, somehow, related. As ω_f decreases, β_e (Eq. (5)) is expected to decrease, whereas $\langle \phi' \nabla P' \rangle$ is expected to increase. A possible explanation is that, as ω_f decreases, the microscopic description of the gas-solid momentum transfer provided by the drag force is progressively replaced by a more macroscopic description. The latter is better understood by reformulating the apparent added mass as an apparent distribution of the filtered gas phase pressure gradient over the phases and an apparent drag force.

ALTERNATIVE FORMULATION FOR THE APPARENT ADDED MASS

By rearranging Eqs. (8) and (9) in a way similar to De Wilde [12], but accounting for the presence of a drag type force, it can be shown that the effect of the meso-scale apparent added mass correction is an apparent distribution of the filtered gas phase pressure gradient over the phases, as already obtained by De Wilde [12], and, additionally, an apparent drag force. Eq. (8) can indeed be rewritten as:

$$\langle\phi\rangle\rho_s\frac{D\langle v\rangle}{Dt}=-\left[\langle\phi\rangle+\frac{C_a\langle\phi\rangle\left(1-\langle\phi\rangle\right)\left(\rho_s-\rho_g\right)\langle\rho_m\rangle}{\langle\phi\rangle\left(1-\langle\phi\rangle\right)\rho_s\rho_g+C_a\langle\rho_m\rangle^2}\right]\nabla\langle P\rangle+\langle\phi\rangle\rho_s g+\left[1-\frac{C_a}{\left(\frac{\langle\phi\rangle\left(1-\langle\phi\rangle\right)\rho_s\rho_g}{\langle\rho_m\rangle^2}\right)+C_a}\right]\beta_e\left(\langle u\rangle-\langle v\rangle\right) \qquad (12)$$

An analogous reformulated equation for the gas phase Eq. (9) can be obtained. The apparent drag force results from the correlation between the solid volume fraction and the gas phase pressure gradient $\langle\phi'\nabla P'\rangle$ and should not be confused with the effective drag force introduced to close the filtered drag force (Eq. (5)). The two can eventually be combined in an apparent effective drag force. As the filter frequency ω_f decreases, C_a is expected to increase and, as seen from Eq. (12), the contribution of the apparent distribution of the filtered gas phase pressure gradient over the phases to the filtered description of gas-solid momentum transfer grows in importance, whereas the contribution of the apparent drag force becomes less important. In case ω_f is low and C_a is large, the distribution of the gas phase pressure gradient over the phases is seen to become (almost) mass fraction based and independent of C_a and the apparent drag is seen to vanish. This limits the solid phase acceleration by gas-solid momentum transfer to the gas phase acceleration, as it should. Hence, as ω_f decreases, the microscopic drag description of the gas-solid momentum transfer is progressively replaced by a more macroscopic description that basically consists of distributing the filtered gas phase pressure gradient, the ultimate macroscopic driving force of both the phases, over the phases.

It should be noted that De Wilde [12] found no evidence for a direct contribution to an apparent drag from the correlation between the solid volume fraction and the gas phase pressure gradient $\langle\phi'\nabla P'\rangle$. Therefore, the possibility of using an apparent distribution of the filtered gas phase pressure gradient over the phases as such, which corresponds to the apparent added mass without the apparent drag force part (Eq. (12)), as a closure model approach for $\langle\phi'\nabla P'\rangle$ could be considered.

The important finding of the reformulation of the apparent added mass in terms of an apparent distribution of the filtered gas phase pressure gradient over the phases and an apparent drag force, on the one hand, and of the mixture speed of sound test showing an unacceptable behavior using the effective drag approach (Figure 1) and an acceptable behavior using the apparent added mass approach (Figure 2), on the other hand, is that an apparent / effective distribution of the filtered gas phase pressure gradient over the phases is able to restore the unacceptable behavior introduced by an apparent / effective drag approach. The apparent added mass approach is in fact doing so, resulting in the acceptable behavior of Figure 2. The combination of an effective / apparent drag force and an effective / apparent distribution of the filtered gas phase pressure gradient over the phases seems, therefore, promising in describing filtered gas-solid momentum transfer.

The 12th International Conference on Fluidization - New Horizons in Fluidization Engineering, Art. 23 [2007]

CONCLUSIONS

Closure models for the filtered gas-solid momentum transfer based on an effective drag approach for the filtered drag force and an apparent added mass approach for the correlation between the solid volume fraction and the gas phase pressure gradient are analyzed. A mixture speed of sound test reveals an unacceptable behavior for the effective drag approach, but an acceptable behavior for the apparent added mass approach. It is shown that the apparent added mass can be reformulated in terms of an apparent distribution of the filtered gas phase pressure gradient over the phases and an apparent drag force. The latter results from the correlation between the solid volume fraction and the gas phase pressure gradient and should not be confused with the effective drag force introduced to close the filtered drag force. The acceptable behavior of the apparent added mass and its reformulation show, however, that an apparent / effective distribution of the filtered gas phase pressure gradient over the phases can compensate for the unacceptable behavior introduced by an apparent / effective drag. A combination of an apparent / effective distribution of the filtered gas phase pressure gradient over the phases and an apparent / effective drag seems, hence, to be a promising way of describing filtered gas-solid momentum transfer. Furthermore, it is shown that, as the filter frequency decreases, the contribution of the apparent / effective distribution of the filtered gas phase pressure gradient over the phases to the filtered description of gas-solid momentum transfer gradually grows in importance up to a mass fraction based distribution, whereas the contribution of the apparent / effective drag force gradually vanishes, the mesoscopic description of gas-solid momentum transfer gradually being replaced by a more macroscopic description.

REFERENCES

1. K. Agrawal, P.N. Loezos, M. Syamlal, S. Sundaresan, *J. Fluid Mech.* 445, 151 (2001).
2. D.Z. Zhang, W.B. VanderHeyden, *Int. J. Multiphase Flow* **28: (5)**, 805 (2002).
3. B.J. Glasser, I. Goldhirsch, *Phys. Fluids* **13:(2)**, 407 (2001).
4. H.T.T. Bi, J.H. Li, *Adv. Powder Technol.* **15:(6)**, 607 (2004).
5. T. Anderson, R. Jackson, *Ind. Eng. Chem. Fundam.* **6**, 527 (1967).
6. J. De Wilde, J. Vierendeels, G.J. Heynderickx, G.B. Marin, *J. Comput. Phys.* **207:(1)**, 309 (2005).
7. C.K.K. Lun, S.B. Savage, D.J. Jeffrey, N. Chepurniy, *J. of Fluid Mech.* **140**:(MAR), 223 (1984).
8. N. Yang, W. Wang, W. Ge, J. Li, *Chem. Eng. J.* **96:(1-3)**, 71 (2003).
9. G.J. Heynderickx, A.K. Das, J. De Wilde, G.B. Marin, *Ind. & Eng. Chem. Res.* **43:(16)**, 4635 (2004).
10. A.T. Andrews, P.N. Loezos, S. Sundaresan, *Ind. & Eng. Chem. Res.* **44:(16)**, 6022-6037 (2005).
11. Y.C. Wen, Y.H. Yu, *Chem. Eng. Progress Symp. Ser.* 62: (62), 100-111 (1966).
12. J. De Wilde, *Physics of Fluids* **17:(11)**, 113304, 14 p. (2005).
13. C.M. Atkinson, H.K. Kytömaa, *Int. J. of Multiphase Flow* 18:(4), 577-592 (1992).
14. W. Gregor, H. Rumpf, *Int. J. of Multiphase Flow* **1:(6)**, 753 (1975).
15. W. Gregor, H. Rumpf, *Powder Technol.* **15:(1)**, 43 (1976).
16. Y.L. Yang, Y. Jin, Z.Q. Yu, Z.W. Wang, *Powder Technol*, **73: (1)**, p. 67-73 (1992).
17. Gillandt I., Fritsching U., Bauckhage K., *Int. J. Multiphase Flow*, **27: (8)**, p. 1313-1332 (2001).